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Good Permutations for Extreme Discrepancy

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The asymptotic behaviour of the discrepancy of the usual van der Corput sequences in arbitrary base b is known; and the implied constants tend to infinity with the base b. The aim of this paper is, first, to prove that for every base b there exist permutations of the digits such that the constants are less than $1/\text{Log}\, 2 = 1.442...$ and, second, to produce a permutation, in base $b = 36$, giving the smallest discrepancy presently known: $\lim\sup(D(N)/\text{Log}\, N) = 23/(35\, \text{Log}\, 6) = 0.366...$.

1. INTRODUCTION

1.1. As usual, for a sequence $X = (x_n)_{n \geqslant 1}$ in $[0, 1]$, let $A(\alpha, N, X)$ be the number of $n \leqslant N$ such that $0 \leqslant x_n < \alpha$, $E(\alpha, N, X) = A(\alpha, N, X) - \alpha N$ and $E([\alpha, \beta[; N, X) = E(\beta, N, X) - E(\alpha, N, X)$, with $0 \leqslant \alpha < \beta \leqslant 1$; the function E is called the remainder.

The *star-discrepancy* is $D^*(N, X) = \sup_\alpha |E(\alpha, N, X)|$, and the *discrepancy* is $D(N, X) = \sup_{\alpha, \beta} |E([\alpha, \beta[; N, X)|$ (in [5], these quantities are divided by N).

Moreover, we introduce the superior limits

$$s^*(X) = \overline{\lim_N}(D^*(N)/\text{Log}\, N) \qquad \text{and} \qquad s(X) = \overline{\lim_N}(D(N)/\text{Log}\, N).$$

By a well-known theorem of W. Schmidt [7], improved by R. Béjian [1], we have $s^*(X) \geqslant 0.06$ and $s(X) \geqslant 0.12$ for every sequence X in $[0, 1]$.

1.2. Given an integer $n \geqslant 1$, write the b-adic representation of $n - 1 = \sum_{j=0}^{\infty} a_j(n)\, b^j$; then, for every permutation σ of the set $B = \{0, 1, ..., b-1\}$, the generalized van der Corput sequence (in fixed base b) S_b^σ is defined by

$$S_b^\sigma(n) = \sum_{j=0}^{\infty} \sigma(a_j(n))\, b^{-j-1}$$

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(we may [4] also define sequences S_b^{Σ} where $\Sigma = (\sigma_j)$ is a sequence of permutations, but this extension is not interesting here).

Note that families of sequences including van der Corput sequences have been constructed by J. P. Borel [2], E. Braaten and G. Weller [3], B. Lapeyre and G. Pagès [6], and A. Thomas [8]; until now, only the last family allows improvements for small discrepancy (see 1.3 below).

1.3. The following theorems state the main results currently known for the van der Corput sequences and their generalizations, according to discrepancy.

THEOREM A [4]. *Let I be the identical permutation; then*

$$s(S_b^I) = s^*(S_b^I) = \begin{cases} b^2/(4(b+1)\operatorname{Log} b) & \text{if } b \text{ is even} \\ (b-1)/(4\operatorname{Log} b) & \text{if } b \text{ is odd.} \end{cases}$$

THEOREM B [4]. *For* $2 \leqslant b \leqslant 20$, *the smallest discrepancy for* S_b^σ *sequences is given by* $b = 12$ *and* $\sigma = (17698)(23\overline{1}\overline{0}45)$ (*product of cycles*) *with* $4828/(5181 \operatorname{Log} 12) = 0.375... \leqslant s(S_{12}^\sigma) < 0.38$.

This was the best result since 1981, before the work of A. Thomas:

THEOREM C [8]. *There exists a sequence* S'_{12}, *in a family containing* S_b^σ *sequences, such that* $s(S'_{12}) \leqslant (4828/5181 - 2 \times 10^{-5})/\operatorname{Log} 12$; *moreover, in Theorem B, the left inequality is an equality.*

1.4. In the present paper we prove two theorems, the first showing that there exist good permutations in any base and the second giving a discrepancy around 0.01 smaller than the preceding ones.

THEOREM 1.1. *For every b there exists σ such that* $s(S_b^\sigma) \leqslant 1/\operatorname{Log} 2$.

Remarks. (1) The permutation σ is obtained by a simple algorithm (see paragraph 3.1).

(2) Compare with Theorem A in which the constants tend to infinity with increasing b.

(3) There is computational evidence that permutations σ from Theorem 1.1 have the property $s(S_b^\sigma) \leqslant 1/(2 \operatorname{Log} 2)$ (checked until $b = 256$); we have not succeeded in our attempts to obtain a demonstration for every b.

THEOREM 1.2. *For* $b = 36$, *the permutation σ defined below gives*

$$s(S_{36}^\sigma) = 23/(35 \operatorname{Log} 6) = 0.3667...;$$

the kth number stands for $\sigma(k)$: (0, 25, 17, 7, 31, 11, 20, 3, 27, 13, 34, 22, 5, 15, 29, 9, 23, 1, 18, 32, 8, 28, 14, 4, 21, 33, 12, 26, 2, 19, 10, 30, 6, 16, 24, 35).

Remarks. (1) We have performed computer programs (Pascal) to investigate best permutations in small base and, when this was done, to calculate the discrepancy and related functions ψ_b^σ (affine functions maxima, see 2.2). So, it was possible to have an intuition of the asymptotic behaviour and to verify the correctness of induction hypotheses.

(2) Unfortunately, for the moment we are not able to develop a process allowing to have better discrepancies with increasing bases b (even for particular b); and bases 12 and 36 are still lucky exceptions... .

2. Basic Formulae on S_b^σ Sequences

2.1. *Functions Related to a Pair* (b, σ) [4, 2.3]

Let $Z_b^\sigma = (\sigma(0)/b, ..., \sigma(b-1)/b)$; for any integer h such that $0 \leqslant h \leqslant b-1$, the function $\varphi_{b,h}^\sigma$ is defined as follows: let k be an integer with $1 \leqslant k \leqslant b$; then for $x \in [(k-1)/b, k/b]$, set

$$\varphi_{b,h}^\sigma(x) = A(h/b, k, Z_b^\sigma) - hx \qquad \text{if} \quad 0 \leqslant h \leqslant \sigma(k-1)$$

and

$$\varphi_{b,h}^\sigma(x) = (b-h)x - A([h/b, 1[; k, Z_b^\sigma) \qquad \text{if} \quad \sigma(k-1) < k < b.$$

The functions $\varphi_{b,h}^\sigma$ are extended to the reals by periodicity; they are continuous and piecewise affine; note that $\varphi_{b,0}^\sigma = 0$.

2.2. *Discrepancy by Means of* φ*-Functions*

The functions $\varphi_{b,h}^\sigma$ give rise to other functions according to the concerned discrepancy; for our purpose, here, we need

$$\psi_b^\sigma = \max_h (\varphi_{b,h}^\sigma) + \max_h (-\varphi_{b,h}^\sigma).$$

Then, the discrepancy of S_b^σ is given by

$$D(S_b^\sigma, N) = \sum_{j=1}^{\infty} \psi_b^\sigma(N/b^j)$$

and

$$s(S_b^\sigma) = \alpha_b^\sigma / \mathrm{Log}\, b \qquad \text{with } \alpha_b^\sigma = \inf_{n \geqslant 1} \sup_{x \in \mathbb{R}} \left(\frac{1}{n} \sum_{j=1}^{n} \psi_b^\sigma(x/b^j) \right)$$

[4, Theorems 1 and 2]; note that the infimum over n is also the limit when n tends to infinity [4, Lemma 4.2.2].

CONSEQUENCE. Set $d_b^\sigma = \max_{1 \leqslant l \leqslant b} \max_{0 \leqslant h < k \leqslant b} |E([h/b, \ k/b[; l, Z_b^\sigma)|$; then $\alpha_b^\sigma \leqslant \sup_{x \in \mathbb{R}} \psi_b^\sigma(x) = d_b^\sigma$ and $d_b^\sigma \leqslant b/4$ [4, 3.2.2]. So $s(S_b^\sigma) \leqslant d_b^\sigma / \operatorname{Log} b$ (see appendix).

2.3. *Intrication* [4, 3.4.3]

Given two pairs (b, σ) and (c, τ) we define a new pair $(bc, \sigma \cdot \tau)$ by the formula

$$\sigma \cdot \tau(l) = c\sigma(h) + \tau(k) \qquad \text{with} \quad l = kb + h, \ 0 \leqslant h \leqslant b-1 \text{ and } 0 \leqslant k \leqslant c-1.$$

PROPERTY. $\psi_{bc}^{\sigma \cdot \tau}(x) = \psi_c^\tau(x) + \psi_b^\sigma(cx)$ and thus $d_{bc}^{\sigma \cdot \tau} \leqslant d_b^\sigma + d_c^\tau$.

3. Proof of Theorem 1.1

3.1. *Construction of the Permutations* σ

For $b = 2$, take $\sigma = I$, the identical permutation. Suppose that (b, σ) is constructed up to $b' = 1$. Then if $b' = 2c$ is even, take $\sigma = \tau \cdot I$ (see 2.3) in which τ is the permutation we have already obtained for the base c. And if $b' = 2c + 1$ is odd, take the permutation σ' obtained from $(2c, \sigma)$, previously constructed, by adding the term $\sigma'(c) = c$ in the middle of σ, and shifting the remaining part; precisely

$$\text{for } 0 \leqslant k < c, \qquad \begin{aligned} &\sigma'(c) = c, \\ &\sigma'(k) = \sigma(k) && \text{if } 0 \leqslant \sigma(k) < c \\ &\sigma'(k) = \sigma(k) + 1 && \text{if } c \leqslant \sigma(k) < 2c \end{aligned}$$

and

$$\text{for } c < k \leqslant 2c, \qquad \begin{aligned} &\sigma'(k) = \sigma(k-1) && \text{if } 0 \leqslant \sigma(k-1) < c \\ &\sigma'(k) = \sigma(k-1) + 1 && \text{if } c \leqslant \sigma(k-1) < 2c. \end{aligned}$$

This construction gives (the kth number stands for $\sigma(k)$)

b	2	3	4	5	6
σ	(01)	(012)	(0213)	(03214)	(024135)

7	8
(0253146)	(04261537)

and so on.

Note that, for $b = 2^a$, this yields the first b points of the original van der Corput sequence in the 2-adic system; note also the symmetry.

3.2. *Lemma*

Let $b' = 2c + 1$; *then* $b'd_{b'}^{\sigma'} \leqslant 2cd_{2c}^{\sigma} + c$.

Proof. Consider the sequence $Z_{b'}^{\sigma'}$ as the set of points $(h, \sigma'(h))$, with $0 \leqslant h \leqslant b' - 1$, in the square $[0, b']^2$. Then by construction, σ' is obtained from σ in the square $[0, 2c]^2$ by adding a new point at the center of the square and shifting correctly the points at the right and under the center.

In this way, $b'E([h/b', k/b'[; l, Z_{b'}^{\sigma'})$ is the number of points, with weight b', belonging to the rectangle $[h, k[\times]0, l]$ minus the rectangle area $(k-h)l$.

If $1 \leqslant l \leqslant c$, we have at most c points in $[k, k[\times]0, l]$; these points come from a rectangle in $[0, 2c]^2$ whose area is equal to $(k-h)l$ (if h and k are both smaller than c or greater then $c+1$) or to $(k-h-1)l$ (in the other case for h and k); each point has weight b' in $[0, b']^2$ instead of $b'-1$ in $[0, 2c]^2$. Therefore the remainder increase is at most c when going from $2c$ to b', because the area is unchanged or greater.

So far we have proved that

$$b'E([h/b', k/b'[; l, Z_{b'}^{\sigma'}) \leqslant 2cd_{2c}^{\sigma} + c.$$

Now, if this remainder is negative, take the complementary rectangle $([0, h] \cup [k, b[) \times]0, l]$, and apply the preceding argument; this yields, for $1 \leqslant l \leqslant c$ and $0 \leqslant h < k \leqslant b'$,

$$b' \, |E([h/b', k/b'[; l, Z_{b'}^{\sigma'})| \leqslant 2cd_{2c}^{\sigma} + c.$$

The case in which $c < l \leqslant b'$ may be treated in the same way; but we can also use the symmetry of $Z_{b'}^{\sigma'}$ with regard to the center of the square; this property gives

$$E([h/b', k/b'[; l, Z_{b'}^{\sigma'}) = -E([1-k/b', 1-b'[; b'-l, Z_{b'}^{\sigma'})$$

and so in any case we get the desired inequality.

3.3. *Proof of Theorem* 1.1

By 2.2, it suffices to prove that $d_{b}^{\sigma}/\text{Log}\, b \leqslant 1/\text{Log}\, 2$. This property is easily verified for small b (even with $1/(2 \,\text{Log}\, 2)$); suppose it is true for all $b' < b$. Then if $b = 2c$, by the property in Section 2.3, we have

$$d_{b}^{\sigma} \leqslant d_{c}^{\tau} + d_{2}^{I}.$$

Therefore

$$\frac{d_b^\sigma}{\operatorname{Log} b} \leqslant \frac{d_c^\tau + d_2^I}{\operatorname{Log} c + \operatorname{Log} 2} \leqslant \max\left(\frac{d_c^\tau}{\operatorname{Log} c}, \frac{d_2^I}{\operatorname{Log} 2}\right) \leqslant \frac{1}{\operatorname{Log} 2}$$

by the induction hypothesis.

Now, if $b = 2c + 1$, from the lemma in Section 3.2, we get

$$d_b^\sigma \leqslant (d_c^\tau + d_2^I)(b-1)/b + c/b, \text{ and so}$$

$$\frac{d_b^\sigma}{\operatorname{Log} b} \leqslant \frac{(b-1)}{b \operatorname{Log} b}\left(\frac{\operatorname{Log} c}{\operatorname{Log} 2} + \frac{1}{2}\right) + \frac{b-1}{2b \operatorname{Log} b}, \qquad \text{with} \quad d_2^I = 1/2;$$

but $\operatorname{Log} c = \operatorname{Log}(b-1) - \operatorname{Log} 2$ and this implies

$$\frac{d_b^\sigma}{\operatorname{Log} b} \leqslant \frac{(b-1)\operatorname{Log}(b-1)}{b \operatorname{Log} b \operatorname{Log} 2} \leqslant \frac{1}{\operatorname{Log} 2} \qquad \text{Q.E.D.}$$

3.4. *Comments*

In view of 2.3, we have always

$$d_{bc}^{\sigma \cdot \tau}/\operatorname{Log}(bc) \leqslant \max(d_b^\sigma/\operatorname{Log} b,\ d_c^\tau/\operatorname{Log} c).$$

So, in addition to 3.1, there are many other ways to obtain good permutations for every base (by intrication if not a prime and else by adding a central point). In many cases one thus gets better results than with 3.1 (for instance with $31 = 6 \times 5 + 1$, we obtain $d_b^{\sigma'} = 58$ and $d_b^{\sigma'}/\operatorname{Log} b = 0.54...$ instead of 67 and 0.62 for the permutation σ of 3.1); but the construction in 3.1 is useful for simplicity and step by step induction.

Our permutations are slightly better than those of Braaten and Weller; see the appendix for comparisons (also with the best permutations we know for $2 \leqslant b \leqslant 20$).

Moreover, the Braaten and Weller construction needs discrepancy computations for each base independently, and they did not try to obtain discrepancy estimates for their sequences; their purpose was numerical multidimensional quasi-Monte-Carlo integration and comparison with Monte-Carlo methods; in this context, they produced permutations for prime bases until 53; we have computed ourselves the estimates in the appendix for these permutations.

We have performed the calculation of $d_b = d_b^\sigma$ (σ as in 3.1) for $2 \leqslant b \leqslant 255$; on the basis of these results, it appears that d_b is maximum in each interval $[2^{k-1}, 2^k[$ for $b_k = 2^k - 1$; more precise estimations give

$$d_{b_k} = \begin{cases} k/2 - 1/3 & \text{if } k \text{ is even} \\ k/2 - 1/3 - 1/(6b_k) & \text{if } k \text{ is odd;} \end{cases}$$

note that $\lim_{k \to \infty}(d_{b_k}/\operatorname{Log} b_k) = 1/(2 \operatorname{Log} 2)$.

So we present the conjecture that

$$d_b/\mathrm{Log}\, b \leqslant 1/(2\,\mathrm{Log}\, 2) \qquad \text{and} \qquad \max_{2^{k-1} \leqslant b \leqslant 2^k} d_b = d_{b_k}.$$

To prove this conjecture, it is probably necessary to investigate carefully the functions ψ_b^σ and especially the relations between ψ_c^τ, $\psi_{2c}^{\tau \cdot I}$ and $\psi_{2c+1}^{\sigma'}$ (see 3.1).

4. Proof of Theorem 1.2

4.1. *Introduction*

As noted in the first remark following the statement of Theorem 1.2, we have found the permutation σ of this theorem by empirical trials relying on computer calculations. So we get d_{36}^σ which gives $s(S_{36}^\sigma) < 0.396$, the best estimation based on $d_b^\sigma/\mathrm{Log}\, b$ (see the appendix), in particular better than the corresponding one for $b = 12$. To go further, it is necessary to compute ψ_{36}^σ and then to evaluate $\sum_{j=1}^{n} \psi_{36}^\sigma(x/36^j)$ (see 2.2); before doing this precisely, we give easily reached upper and lower bounds, showing that the constant $s(S_{36}^\sigma)$ is really the best one (with regard to Theorems B and C).

4.2. *Proposition*

Proposition. *The function ψ_{36}^σ resulting from the permutation σ is given by Table I; the kth line contains one, two, or three affine functions given by*

TABLE I

k	First function		Second function		Third function	
1	0	35	—	—	—	—
2	35	34	24	48	—	—
3	48	36	32	48	—	—
4	48	28	45	36	30	40
5	40	32	36	45	32	49
6	49	30	48	36	35	42
7	42	37	30	47	—	—
8	47	28	44	40	33	48
9	48	36	40	45	—	—
10	45	42	27	46	—	—
11	46	29	38	49	30	51
12	51	36	41	48	—	—
13	48	40	36	48	24	50
14	50	40	42	48	31	50
15	50	33	42	45	—	—
16	45	24	27	48	—	—
17	48	33	40	47	24	48
18	48	36	—	—	—	—

their values at the ends of the intervals $[(k-1)/36, k/36]$; *on such an interval,* ψ_{36}^{σ} *is the supremum of these functions; the computation shows that* $\psi_{36}^{\sigma}(x) = \psi_{36}^{\sigma}(1-x)$ *for* $x \in [1/2, 1]$, *so the table ends with* $k = 18$.

Proof. The only thing we have to do is to apply formulae in Sections 2.1 and 2.2; this may be achieved by hand, pencil and rule, or by a computer program; we have performed both methods and we have obtained the same result.

4.3. *Upper and Lower Bounds*

We follow the method developed in [4, 5.2],

$$\text{set } F_n(x) = \sum_{k=0}^{n-1} \psi(xb^k); \text{ then } \alpha = \inf_{n \geqslant 1} \big(\max_{x \in [0,1]} F_n(x)/n \big),$$

and to obtain an upper bound, it is sufficient to compute $d_n = \max F_n(x)$ for $1 \leqslant n \leqslant n_0$ with fixed n_0. For $n_0 = 4$, we get $\alpha_{36}^{\sigma} < 1 \cdot 33882$ (reached with $x = 515882/36^4$) and this bound gives $s(S_{36}^{\sigma}) < 0.37361$.

To obtain a lower bound, we compute $(1/\nu) F_\nu(a/(b^\nu - 1))$ for given integers a and ν so that $1 \leqslant a \leqslant b^\nu$ (see [4, 5.2.1] for justification); with $\nu = 1$ and $a = 2$ we get $s(S_{36}^{\sigma}) \geqslant 0.3667... = 23/(35 \operatorname{Log} 6)$; this is the value to be obtained for $s(S_{36}^{\sigma})$ by exact calculation.

At present, we therefore have

$$0.3667 < s(S_{36}^{\sigma}) < 0.37361.$$

4.4. *Exact Calculation of* $s(S_{36}^{\sigma})$

We apply [4, 5.3–5.4] and the dominated interval notion: let $I_h^n = [h/b^n, (h+1)/b^n]$; the interval I_h^n is called *dominated* if there exists a set J of integers with $h \notin J$ such that $F_n(x) \leqslant \max_{j \in J} F_n(x + (j-h)/b^n)$ for all $x \in I_h^n$; an interval is called *dominant* if it is not dominated.

In fact one may work with half-intervals when the function ψ is symmetric, that is, with intervals $J_h^n = [h/b^n, (h+1/2)\, b^n]$, h integer or half-integer.

In the present case, there are two dominant half-intervals J_{11}^1 and J_{13}^1 for $n = 1$, and one dominant half-interval, J_{398}^2, for $n = 2$.

Then numerical investigations lead to the following induction hypothesis: There is only one dominant half-interval $J_{h_n}^n$ for every $n \geqslant 2$, given by

$$h_n = 11 \times 36^{n-1} + 2(36^{n-1} - 1)/35.$$

On this half-interval, F_n is the affine function $p_n(x-h_n/36^n)+q_n$ with

$$p_n = -15 - \frac{12\times 36}{35}\,(36^{n-1}-1),$$

$$q_n = n\,\frac{46}{35} + \frac{481}{4\times 35^2} + \frac{31}{35^2\times 6^3\times 36^{n-2}},$$

and $\max_{x\in J^n_{h_n}} F_n(x) = q_n$.

It remains to add $\psi(xb^n)$ to $F_n(x)$ on $J^n_{h_n}$ and to check that the induction hypothesis is true for F_{n+1}. First we compute F_{n+1} on $J^{n+1}_{h_{n+1}}$ and find effectively $p_{n+1}(x-h_{n+1}/36^{n+1})+q_{n+1}$, because, as is easily seen, $h_{n+1}=36h_n+2$, $p_{n+1}=p_n-12\times 36^n$, and $q_{n+1}=q_n+2p_n/36^{n+1}+48/36$. Then we compare this affine function with the other affine functions given by the other intervals ($36h_n+k$ with $0\leqslant k\leqslant 18$, $k\neq 2$) and check in each case that $J^{n+1}_{h_{n+1}}$ is dominant.

Therefore we have proved that $d_n=\max_{x\in[0,1]} F_n(x)=q_n$ and so $\alpha^\sigma_{36}=\inf_{n\geqslant 1} d_n/n=\lim_{n\to\infty} d_n/n=46/35$; Theorem 2.1 is proved.

TABLE II

b	bd^I_b	bd^τ_b	bd^σ_b	$bd^{\sigma_0}_b$	$d^I_b/\mathrm{Log}\,b$	$d^\tau_b/\mathrm{Log}\,b$	$d^\sigma_b/\mathrm{Log}\,b$	$d^{\sigma_0}_b/\mathrm{Log}\,b$
2	1	1	1	1	0.72	0.72	0.72	0.72
3	2	2	2	2	0.60	0.60	0.60	0.60
4	4	—	3	3	0.72	—	0.54	0.54
5	6	4	4	4	0.74	0.49	0.49	0.49
6	9	—	6	6	0.83	–	0.55	0.55
7	12	8	8	6	0.88	0.58	0.58	0.44
8	16	—	9	8	0.96	—	0.54	0.48
9	20	—	9	9	1.01	—	0.45	0.45
10	25	—	12	10	1.08	—	0.52	0.43
11	30	15	13	13	1.13	0.56	0.49	0.49
12	36	—	16	12	1.20	—	0.53	0.40
13	42	20	19	15	1.25	0.59	0.56	0.44
14	49	—	21	16	1.32	—	0.56	0.43
15	56	—	25	18	1.37	—	0.61	0.44
16	64	—	23	19	1.44	—	0.51	0.42
17	72	29	26	21	1.49	0.60	0.53	0.43
18	81	—	24	22	1.55	—	0.46	0.42
19	90	33	27	25	1.60	0.58	0.48	0.44
20	100	—	30	25	1.66	—	0.50	0.41
31	240	66	67	—	2.25	0.61	0.62	—
36	324	—	60	51	2.51	—	0.46	0.39

Note. We have kept only the first two digits.

APPENDIX

In this appendix, we denote by I the identity, by τ the Braaten–Weller permutations, by σ our permutations (3.1), and by σ_0 the best permutations (known to 20). See Section 2 for the meaning of d_b^σ (Table II).

Note that Braaten and Weller needed only prime bases for their purpose, but their construction runs for every base.

We have computed the table values for their sequences, but we do not know general estimates.

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